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13. ABSTRACT *(Maximum 200 words)*

Research efforts and achievements in the area of modeling and computational methods in distributed parameter physical systems are summarized. Significant progress is reported on projects involving (i) modeling of hepatic uptake and elimination of dioxin, (ii) modeling and parameter estimation in electromagnetic field/solid interactions, and (iii) radio frequency bonding of adhesives.

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FINAL TECHNICAL REPORT

for the period

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Executive Summary

We have carried out research in the modeling and inverse problems for specific physical and biological distributed parameter (partial differential equation) systems. Our efforts involved theoretical, computational, and in some cases, experimental aspects of the problems addressed. As part of our modeling efforts, specific inverse or parameter estimation problems were investigated.

A major thrust of our work involved research on health sciences related issues of interest to the Air Force and is collaborative with scientists in the AFRL, Brooks AFB. Specific topics investigated include control of electromagnetic signals in dispersive media, and advanced pharmocodynamic modeling as a component of a computational therapeutic modeling methodolog. In dual use type efforts, a collaborative project with Lord Corp. on the use of electromagnetic signals at radio frequency to cure adhesives in commercial bonding processes was investigated.

Student investigators supported under this grant have made significant progress in the past 3 years on several topics. These can be roughly divided into several distinct but related areas: (i) modeling of hepatic uptake and elimination of dioxin, and (ii) estimation of electromagnetic dispersion and geometry using incident microwave pulses, and (iii) process control systems for radio frequency curing of adhesive bonding in composite structures. The research efforts on the first two subjects are in close collaboration with Dr. Richard Albanese and associates in Armstrong Labs (now AFRL), Mathematical Products Division, Brooks Air Force Base. Detailed descriptions of the efforts and results can be found in the readily available publications listed in this report. Those listed as CRSC-TR are technical reports available from the Center for Research in Scientific Computation at North Carolina State University. Among investigators supported in part under this grant are C. Musante (Ph.D. thesis completed in May, 1998), M. Buksas (Ph.D. thesis to be completed in August, 1998) and M. Goodhart (completion of Ph.D. thesis anticipated in Spring, 1999).

I. Modeling the Hepatic Uptake and Elimination of 2,3,7,8- Tetrachlorodibenzo-p-dioxin

The objective of our research was the development of advanced pharmacokinetic modeling techniques to describe the transport of solutes within the liver. Our particular interest is the chemical compound 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). TCDD enters in the environment through combustion sources such as the burning of municipal and hospital wastes and in the production of certain herbicides. In particular, TCDD is an unwanted by- product in the manufacture of 2,4,5-trichlorophenoxyacetic acid (2,4,5-T) which was a primary component of Agent Orange used by U.S. forces during the Vietnam conflict. A number of studies have been conducted to determine possible adverse health effects in Vietnam-era veterans who may have been exposed to Agent Orange. Of particular concern to researchers is TCDD's ability to produce a wide range of effects in animals following exposure, including certain types of cancer.

Physiologically-based pharmacokinetic models which have attempted to describe the hep-

atic uptake, distribution, and elimination of TCDD have generally used the well- stirred or venous-equilibrium model to describe events occurring in the liver. The basic assumption of this model, that the concentration of solute is uniform throughout the length of the liver acinus, does not describe the elimination of solutes with decreasing concentration gradients along the acinus following a bolus input. In addition, the "well- stirred" model cannot accommodate spatial variations in other parameters, such as enzyme activity and hepatic cell permeability.

We have developed a convection-dispersion model for the hepatic uptake and elimination of TCDD. This model incorporates the complex architecture and physiology of the human liver and includes the dynamics of TCDD interaction with two intracellular proteins, the Ah receptor and cytochrome P450 1A2 [2]. The resultant mathematical model is a nonlinear coupled system of partial differential equations and ordinary differential equations with time delay. We have established the well-posedness of the model [3], have developed approximation methodologies (with convergence arguments) for numerical simulation and the inverse problem, and are continuing initial promising simulation findings. A summary of theoretical and numerical results to date is given in the Ph.D. thesis of Musante [4].

II. Estimation of Dielectric Parameters and Geometry in Electromagnetic Dispersion

Microwave images of tissue structures and soils play very important roles in many areas, including clinical and environmental medicine. These microwave images are useful in detection/enhanced treatment of abnormality of human organs and tissue, and detection/remediation of underground toxic wastes. The electromagnetic properties of a medium are generally characterized by its electric and magnetic polarization mechanisms and its static conductivity. Our recent efforts involved the development of partial differential equation (Maxwells equations) based identification techniques for dispersion in physical and biological distributed parameter systems, with those for living tissue being a special case.

Our efforts have focused on a time domain approach for the investigation of dispersion mechanisms of a medium in electromagnetic field problems. We use Maxwells equations coupled with a generalized electric polarization model in terms of a convolution of the electric field with an impulse response function. This model includes time hysteresis mechanisms as well as the usual ordinary differential equations (e.g. Debye, Lorentz and multiples of these) for dispersion. Existence, uniqueness and continuous dependence of solutions on data have been given for a one-dimensional (p-polarized plane waves) dispersive medium case in [5, 6]. Estimation of electromagnetic properties of media have been demonstrated via numerical examples. Parameters representing the electromagnetic property of a medium may include the static permittivity, relaxation time, natural frequency, static conductivity, etc. depending on the polarization model chosen.

The methodology for estimation of electromagnetic parameters has also been used as a basis for interrogation of geometry of targets. Computational efforts based on "method of mappings" techniques used in optimal shape design have verified the ability to use electromagnetic pulse probes to determine geometry as well as material dielectrics when the

interrogated body has partial boundaries of supraconductive material [6]. We have recently [7] demonstrated the possiblity of use of acoustic gratings in place of the supraconductive back boundary as a reflector of electromagnetic probes in determining geometry. These results are a direct extension of the inverse algorithms developed in [6]. As a part of his thesis research effort, Buksas has developed a user friendly C++ software package for general polarization model simulation and estimation problems. His thesis is near completion (expected date of August, 1998).

III. Electromagnetic Curing of Adhesives

Modeling of the nonlinear heating process for radiofrequency bonding of adhesives involving electromagnetic heating, exothermic reaction of the adhesives and non-linear diffusion and cooling has been investigated in theoretical, computation, and experimental efforts. Details are reported in a just completed manuscript [8]. A major new component involves the study of the radio frequency input term based on reasonable polarization assumptions in the structural member component [9]. These efforts are the thesis research of M. Goodhart. Excellent progress has been made and her thesis should be completed in Spring, 1999.

IV. Interactions and Transitions

Under support of this AASERT grant for graduate students and the parent grant, substantial interactions and collaborations with Air Force scientists took place during the period of funding.

In the earlier part of the funding period, numerous collaborations with Dr. Richard Albanese and his associates, including Dr. Yun Wang, at Armstrong Labs, Brooks AFB, occured in the areas of electromagnetic dispersion and hepatic modeling of dioxin. Specific detailed collaborations occured during the following dates:

1995: Jan. 19-23 (Albanese and Wang); Feb. 22-24 (Blaschak and Wang); April 27-29 (Wang); July 13-14 (Wang); Aug. 28-30 (Wang); Oct. 26-29 (Albanese and Wang); Dec. 15-16 (Wang).

1996: April 27-30 (Albanese and Wang); June 17-19 (Wang); July 30-31 (Albanese); Aug. 6-10 (Wang); Sept. 19-21 (Albanese, Wang, Blaschak, Medine).

1997: Jan. 3-8 (Albanese); May 5-7 (Albanese).

A number of theses visits involved Banks, Musante and Buksas in visits to Brooks Air Force Base.

The collaborations intensified during 1997 with the following visits:

1. June 15-August 30, 1997: C. Musante, a graduate student at NCSU, spent a 10 week summer fellowship with Albaneses group at Brooks AFB. Substantial progress was made on modeling and simulation of dioxin transport in the liver.

2. July 30-August 2, 1997: H.T. Banks visited and collaborated with Albanese and group at Brooks Air Force Base. In addition to discussions of the dioxin efforts, our progress on inverse imaging and interrogation using electromagnetic probes was discussed.

3. November 13, 1997: H.T. Banks and C. Musante visited with Jeff Fisher and colleagues in the toxicology group at Wright Patterson to discuss our progress in the dioxin modeling project.

The AFOSR supported research in this grant has led to specific and multiple collaborations with scientists at Lord Corporation (Dr. Lynn Yanyo, Dr. Beth Muñoz, Dr. Mark Jolly, Scott Durso, and Mike Gaitens among others). Enabling research has led to development of computational methodologies and software packages for several inverse problems involving distributed parameter systems. Projects on elastomers and magnetorheological fluids have used direct transitions of ideas developed in the context of AFOSR support through this grant. Specific application of ideas has been made in the modeling and design of rubber based elastomers to be used in automotive, aircraft, and heavy equipment vibration suppression devices. Details of some of these results are included throughout the numerous publications listed as partially supported by the parent grant (see Final Technical Report for F49620-95-1-0236).

VI. Publications Supported in Part Under this Grant

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[3] H.T. Banks and C.J. Musante, "Well-posedness for a Class of Abstract Nonlinear Parabolic Systems with Time Delay," CRSC-TR97-30, September, 1997; *Nonlinear Analysis: Theory, Methods and Applications*, to appear.

[4] C.J. Musante, "A Distributed Parameter Model for Spatially Dependent Hepatic Processing of 2,3,7,8-TCDD,"Ph.D. Thesis, North Carolina State University, May, 1998.

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[6] H.T. Banks and M. Buksas, "Electromagnetic Interrogation of Dielectric Materials", in preparation.

[7] H.T. Banks and T. Lin, " Determining the Structure of Biological Media Using Acousto-optic Probes", CRSC TR98-21, May, 1998; *J. Inverse and Ill-Posed Problems*, submitted.

[8] H.T. Banks, S.R. Durso, M.A. Goodhart and K. Ito, "Nonlinear Exothermic Contributions to Radio Frequency Bonding of Adhesives," CRSC-TR98-24, June, 1998; *SIAM J. Sci. Comp.*, submitted.

[9] H.T. Banks, S.R. Durso, M.A. Goodhart and M.L. Joyner, "On the Radio Frequency Inputs in Dipolar Heating of Adhesives," CRSC-TR98-3, January, 1998; *J. Microwave Power and Electromagnetic Energy*, submitted.